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Title: Salts in Hot Water: Developing a Scientific Basis for Supercritical
Desalination and Strategic Metal Recovery

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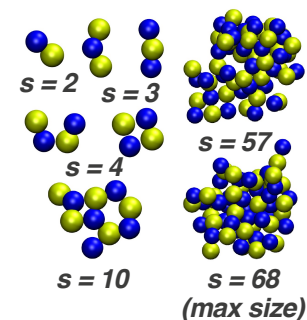
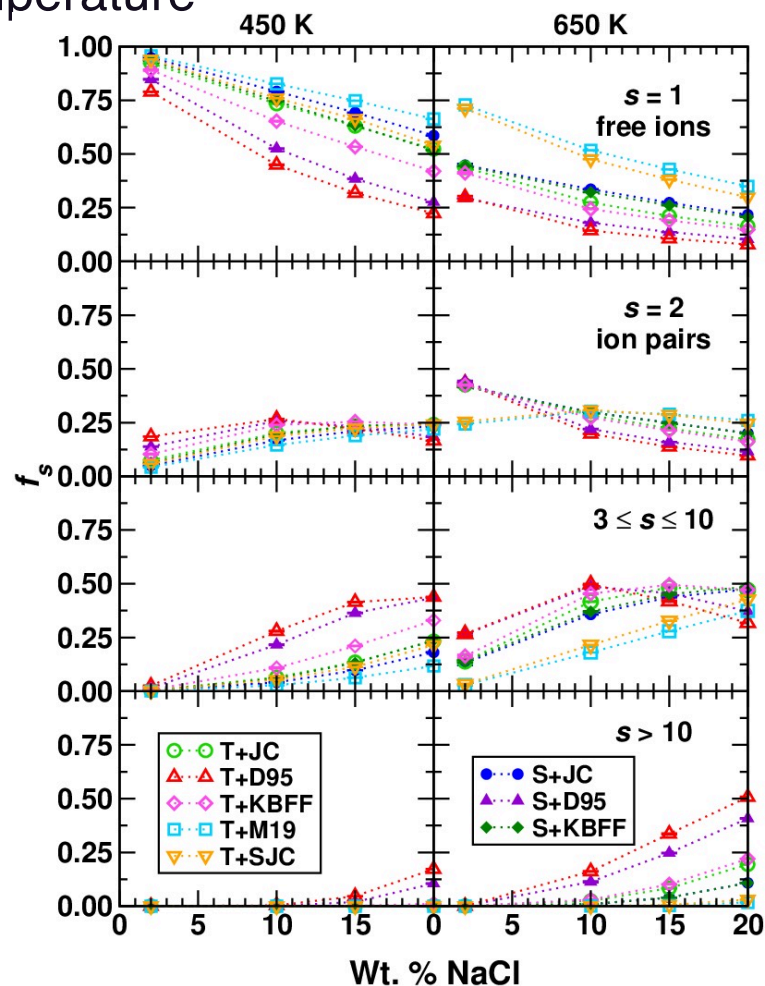
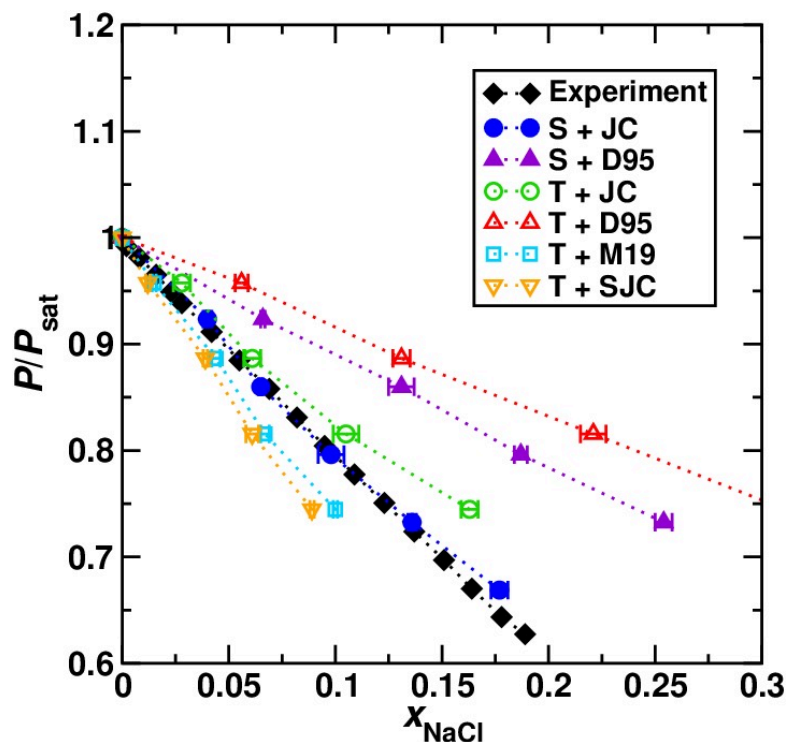
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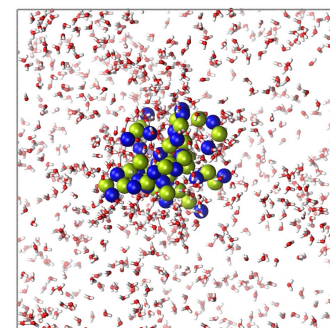
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Comparison of Classical Force Fields

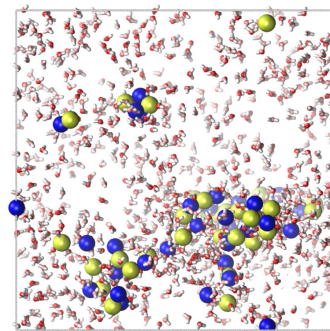
- Evaluate combinations of water and NaCl force fields to see how they behave at high temperatures
 - the general trend is an increasing fraction of molecules in clusters with increasing temperature
 - S + JC does best at predicting pressure-composition isotherms



S + JC

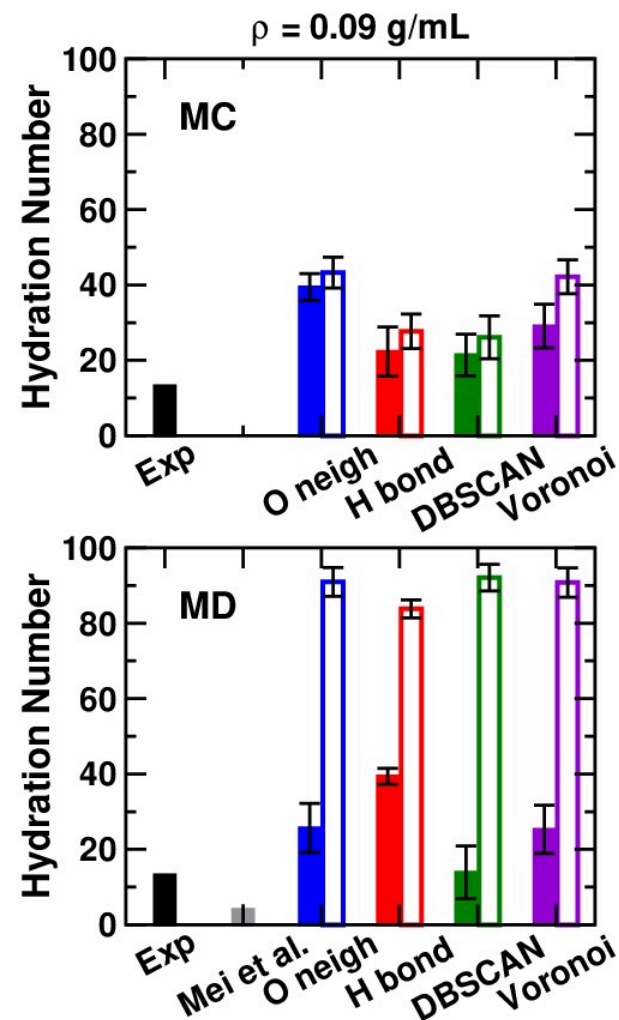
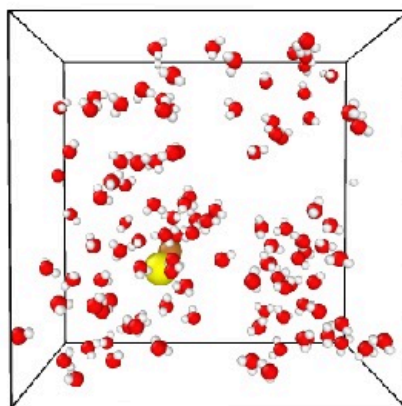
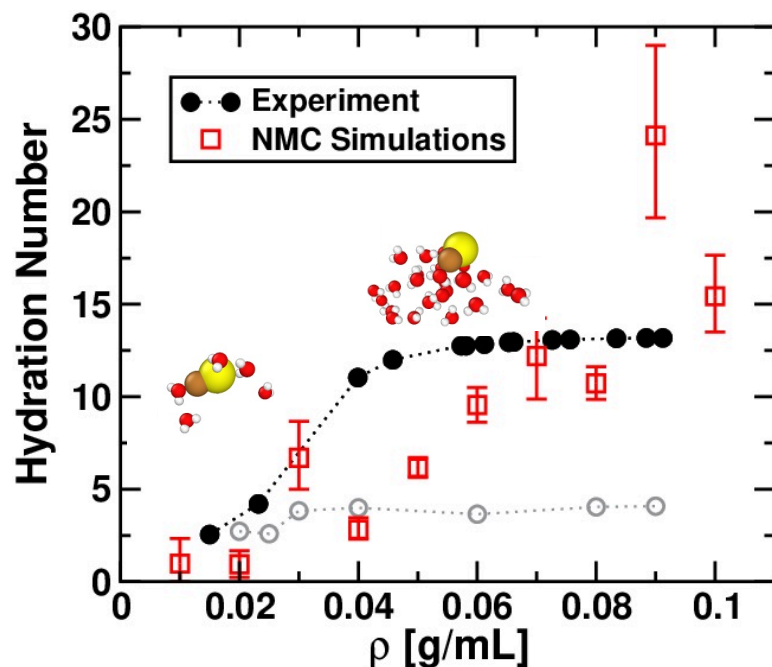


T + M19



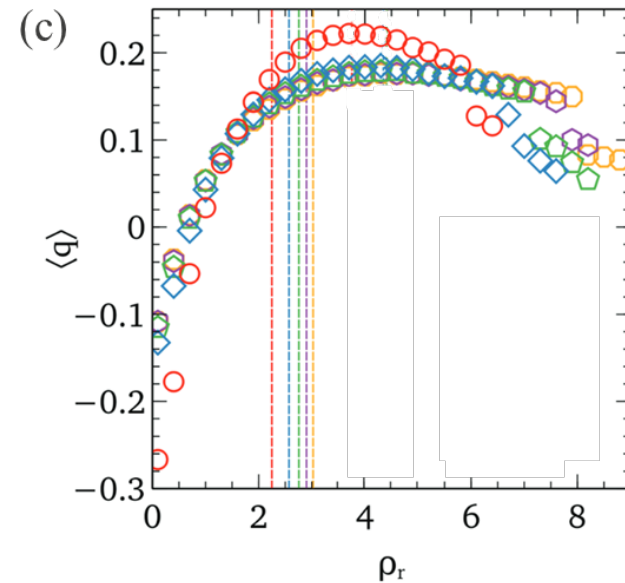
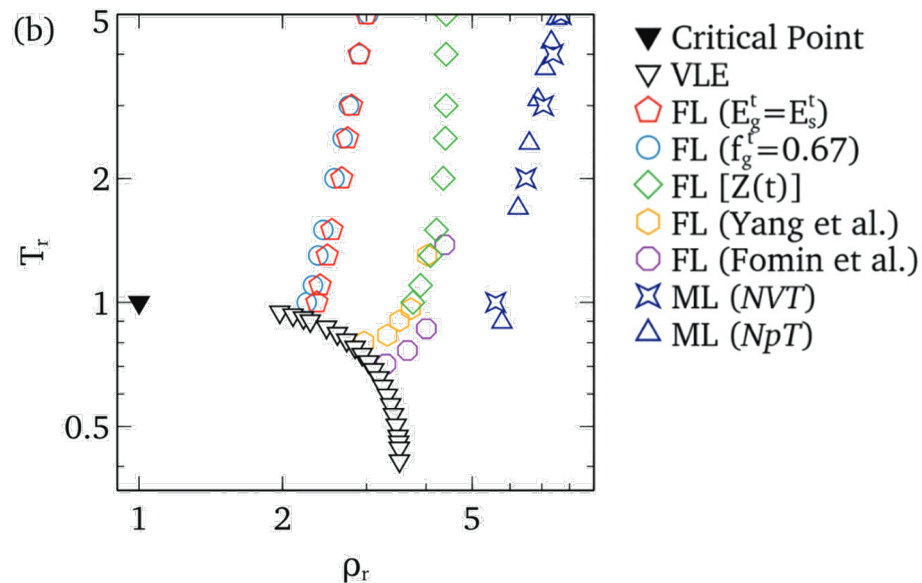
High Temperature Aqueous CuCl Vapors

- Aqueous vapor and low-density supercritical fluids play an important role in metal transport in the earth
 - solubility of metals in these high-temperature vapors is controlled by the formation of hydrated clusters
- First principles MD and MC simulations
 - MD simulations don't sample equilibrium configurations; pronounced system size effects
 - MC simulations with specialized cluster moves are the better method



Supercritical Water at Extreme Conditions

- Will water act like “water” under supercritical conditions?
- Use MD simulations to determine the Frenkel line (FL)
 - set of thermodynamic states that divide the fluid region into gas-like and solid-like
 - parallelism between the melting line and Frenkel line



- Supercritical water becomes an (almost) simple fluid
 - thermodynamic scaling, vanishing tetrahedrality (q ; $q=0.67$ for ambient water))
- High-temperature plastic crystal (non-zero rotational diffusion)